

F/S INTERFACES: POINT CONTACT VERSUS ATOMIC THICKNESS GEOMETRIES

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We contrast perturbative expansions of ferromagnet / superconductor interfaces in two geometries: (i) a point contact geometry where a single weak link connects a 3D ferromagnet to a 3D superconductor and (ii) an atomic thickness geometry with an infinite planar interface connecting a quasi-2D ferromagnet to a quasi-2D superconductor. Perturbation theories are rather different in the two approaches but they both break down at order t^4 (t is the tunnel amplitude). The regimes of strong ferromagnets are in a qualitative agreement in both geometries. The regime of weak ferromagnets exists only for the atomic thickness geometry and is related to Andreev bound states due to lateral confinement in the superconductor.

1 Introduction

Many recent works have been devoted to equilibrium properties of ferromagnet / superconductor (F/S) interfaces, which consists in determining the value of the self-consistent superconducting gap as a function of the various parameters. For instance it was shown that the critical temperature of F/S superlattices is reentrant as a function of the exchange field^{1,2} and that the critical temperature of F/S bilayers is reentrant as a function of the thickness of the ferromagnet^{3,4,5}. Other predictions were made recently within a model where the superconductor is connected by a single weak link to a ferromagnet⁶: it was shown within this model that the superconducting gap of a F/S/F trilayer in the parallel alignment is larger than in the antiparallel alignment⁷, a result that was also obtained within a model of F/S/F trilayer with atomic thickness and half-metal ferromagnets⁸ that was finally extended to Stoner ferromagnets⁹. The goal of this note is to compare the perturbative expansions in the two approaches (point contact versus atomic thickness geometries).

2 Point contacts

2.1 The model

Let us consider a three dimensional (3D) ferromagnet described by the Stoner model connected by a single link to a 3D superconductor described by the BCS Hamiltonian (see Fig. 1-(a)). The Hamiltonian takes the form $\mathcal{H} = \mathcal{H}_{\text{BCS}} + \mathcal{H}_{\text{Stoner}} + \mathcal{W}$, where the BCS Hamiltonian is given by $\mathcal{H}_{\text{BCS}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \Delta \sum_{\mathbf{k}} (c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k},\downarrow}^{\dagger} + c_{\mathbf{k},\downarrow} c_{-\mathbf{k},\uparrow})$, the Stoner Hamiltonian is given by $\mathcal{H}_{\text{Stoner}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} - h_{\text{ex}} \sum_{\mathbf{k},\sigma} (c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k},\uparrow} - c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k},\downarrow})$ and the tunnel Hamiltonian is given by $\mathcal{W} = t \sum_{\sigma} (c_a^{\dagger} c_a + c_a^{\dagger} c_{\alpha})$ where α and a are neighboring sites belonging to the superconductor and ferromagnet respectively.

2.2 Green's functions

For the point contact model we use the Green's functions in real space:

$$\hat{g}(R, \omega) = \frac{2m}{\hbar^2} \frac{1}{2\pi R} \exp\left(-\frac{R}{\xi(\omega)}\right) \left\{ \frac{\sin(k_F R)}{\sqrt{\Delta^2 - \omega^2}} \begin{bmatrix} -\omega & \Delta \\ \Delta & -\omega \end{bmatrix} + \cos(k_F R) \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \right\}, \quad (1)$$

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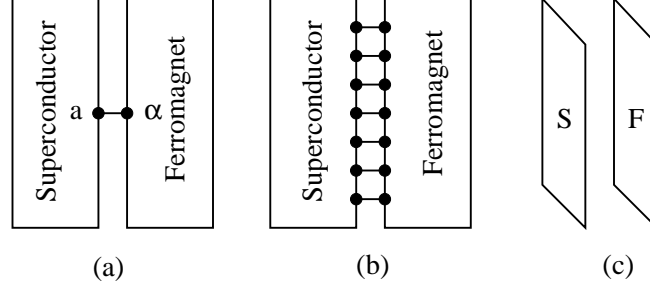


Figure 1: (a) Schematic representation of different types of ferromagnet / superconductor contacts. In (a) a 3D ferromagnet and a 3D superconductor are connected by a single weak link⁷. In (b) a 3D ferromagnet and a 3D superconductor are connected by an infinite planar contact⁷. In (c) an atomic thickness 2D ferromagnet is connected to an atomic thickness 2D superconductor by an infinite planar contact^{8,9,10}.

where $\xi(\omega) = \hbar v_F / \sqrt{|\Delta^2 - \omega^2|}$ is the coherence length at a finite frequency, Δ is the superconducting gap and k_F is the Fermi wave-vector. The local propagator $\hat{g}_{\text{loc}}(\omega)$ is regularized by introducing an ultra-violet cut-off R_0 :

$$\hat{g}_{\text{loc}}(\omega) = \frac{m}{\pi \hbar^2} \begin{bmatrix} -k_F \omega / \sqrt{\Delta^2 - \omega^2} - 1/R_0 & k_F \Delta / \sqrt{\Delta^2 - \omega^2} \\ k_F \Delta / \sqrt{\Delta^2 - \omega^2} & -k_F \omega / \sqrt{\Delta^2 - \omega^2} + 1/R_0 \end{bmatrix}. \quad (2)$$

2.3 Expansion of the magnetization in the superconductor

The fully dressed Green's function $\hat{G}_{x,x}$ in the superconductor is obtained through the Dyson equation $\hat{G}_{x,x} = \hat{g}_{x,x} + \hat{g}_{x,\alpha} \hat{t}_{\alpha,a} \hat{g}_{a,a} \hat{t}_{a,\alpha} \hat{G}_{\alpha,x}$, where $\hat{G}_{\alpha,x}$ is determined through $\hat{G}_{\alpha,x} = \hat{g}_{\alpha,x} + \hat{g}_{\alpha,\alpha} \hat{t}_{\alpha,a} \hat{g}_{a,a} \hat{t}_{a,\alpha} \hat{G}_{\alpha,x}$. The magnetization $m(\omega)$ induced in the superconductor is defined as the difference between the spin-up and spin-down density of states. We find the expansion $m(\omega)/h_{\text{ex}} = A^{(2)}(\omega)t^2 + A^{(4)}(\omega)t^4 + \dots$, with

$$A^{(2)}(\omega) = \frac{m^4}{\pi^4 \hbar^6 k_F R^2} \exp\left(-\frac{2R}{\xi(\omega)}\right) \left\{ \cos(2k_F R) + \frac{\omega}{\sqrt{\Delta^2 - \omega^2}} \sin(2k_F R) \right\} \quad (3)$$

$$A^{(4)}(\omega) = \frac{m^6}{\pi^6 \hbar^{10} R_0 R^2} \exp\left(-\frac{2R}{\xi(\omega)}\right) \left\{ \frac{\omega}{\sqrt{\Delta^2 - \omega^2}} \cos(2k_F R) - \sin(2k_F R) \right\} \quad (4)$$

$$+ \frac{m^6}{\pi^6 \hbar^{10} k_F R_0^2 R^2} \exp\left(-\frac{2R}{\xi(\omega)}\right) \left\{ \cos(2k_F R) + \frac{\omega}{\sqrt{\Delta^2 - \omega^2}} \sin(2k_F R) \right\}. \quad (5)$$

The second order term shows $2k_F$ Friedel oscillations and does not depend on the ultra-violet cut-off R_0 . The fourth order terms are divergent if the ultra-violet cut-off R_0 tends to zero.

We find a similar expansion for $\omega > \Delta$. The structure of the expansion is given by

$$A^{(2)}(\omega) = \frac{m^4}{\pi^4 \hbar^6 k_F R^2} \left\{ \cos(2k_F R) \cos\left(\frac{2R}{\xi(\omega)}\right) - \frac{\omega}{\sqrt{\omega^2 - \Delta^2}} \sin(2k_F R) \sin\left(\frac{2R}{\xi(\omega)}\right) \right\} \quad (6)$$

$$A^{(4)}(\omega) = \frac{m^6}{\pi^6 \hbar^{10}} \left\{ \frac{k_F}{R^2} A_0^{(4)} + \frac{1}{R_0 R^2} A_1^{(4)} + \frac{1}{k_F R_0^2 R^2} A_2^{(4)} \right\}, \quad (7)$$

where we obtained the explicit expression of $A_0^{(4)}$, $A_1^{(4)}$ and $A_2^{(4)}$. The perturbative expansion breaks down since the final result is diverging in the limit $R_0 \rightarrow 0$. The divergences can be removed empirically by interpreting R_0 as an extra integration variable in the fourth order diagrams. The diverging prefactors cancel once the integration over R_0 is carried out. For example $A^{(4)}(\omega)$ in (5) and (7) is replaced by $\int_0^{1/k_F} 4\pi R_0^2 A^{(4)}(\omega) dR_0$. However the proportionality factor in the upper bound of the integral over R_0 remains arbitrary.

2.4 Expansion of the Gorkov function

The superconducting gap is determined self-consistently through the relation

$$\Delta_{\mathbf{x}} = U \int_0^D \frac{d\omega}{2\pi} \text{Im} \left[G_{\mathbf{x},\mathbf{x}}^{1,2,A}(\omega) \right], \quad (8)$$

where U is the microscopic attractive interaction, D is the band-width and $G_{\mathbf{x},\mathbf{x}}^{1,2,A}(\omega)$ is the advanced “12” component of the Green’s function. The expansion of the Gorkov function is given by $G_{1,2}(\omega) = g_{1,2}(\omega) + B^{(2)}(\omega)t^2 + B^{(4)}(\omega)t^4 + \dots$, with

$$g_{1,2}(\omega) = \frac{k_F m \Delta}{\pi \hbar^2 \sqrt{\omega^2 - \Delta^2}} \quad (9)$$

$$\text{Im} \left[B^{(2)}(\omega) \right] = -\frac{m^3 \Delta}{\hbar^6 \pi^3 R^2} \left[\frac{k_F \omega}{\omega^2 - \Delta^2} \sin^2(k_F R) - \frac{1}{2R_0 \sqrt{\omega^2 - \Delta^2}} \sin(2k_F R) \right]. \quad (10)$$

Averaging over oscillations at scale $\lambda_F = 2\pi/k_F$ we obtain the average value of $B^{(2)}(\omega)$:

$$\text{Im} \left[\overline{B^{(2)}(\omega)} \right] = -\frac{m^3 \Delta k_F}{2\hbar^6 \pi^3 R^2} \frac{\omega}{\omega^2 - \Delta^2}. \quad (11)$$

The integral over ω of $g_{1,2}(\omega) + B^{(2)}(\omega)t^2$ is diverging logarithmically and the superconducting gap is reduced at order t^2 . At order t^4 we obtain the average value of $B^{(4)}(\omega)$:

$$\text{Im} \left[\overline{B^{(4)}(\omega)} \right] = \frac{m^7 \Delta}{\hbar^{10} \pi^5 k_F R^2} \left[\frac{\omega^3(\omega + 2h_{\text{ex}})}{(\omega^2 - \Delta^2)^{3/2}} - \frac{2\omega h_{\text{ex}}}{\sqrt{\omega^2 - \Delta^2}} \right] + \dots \quad (12)$$

The perturbative expansion of the self-consistent superconducting gap at order t^4 breaks down since $\overline{B^{(4)}(\omega)}$ grows like ω . Therefore the integral over ω in (8) diverges faster than logarithmically.

3 Bilayers and trilayers with atomic thickness

Let us consider now infinite planar F/S interfaces^{8,9,10}. For simplicity we restrict the discussion to F/S bilayers and F/S/F trilayers with atomic thickness (see Fig. 1-(c)). We use the labels “a” and “b” for the two ferromagnets and the label “ α ” for the superconductor. For strong ferromagnets ($\Delta_0 \ll t \ll h_{\text{ex}}$) the perturbative expansion to order t_a^2 and t_b^2 takes the form⁹

$$\ln \left(\frac{\Delta}{\Delta_0} \right) = -2 \frac{t_a^2 + t_b^2}{h_{\text{ex}}^2} \left[\ln \left(\frac{h_{\text{ex}}}{\Delta_0} \right) - \frac{1}{2} \right], \quad (13)$$

where Δ_0 is the superconducting gap of the isolated superconductor. For weak ferromagnets ($t \ll h_{\text{ex}} < \Delta_0$) we find⁹

$$\ln \left(\frac{\Delta}{\Delta_0} \right) = -\frac{1}{2} \frac{(t_a^2 + t_b^2) h_{\text{ex}}^2}{\Delta_0^4}. \quad (14)$$

At order t^4 the superconducting gap Δ_P in the parallel alignment is different from the superconducting gap Δ_{AP} in the antiparallel alignment. For strong ferromagnets we find⁹

$$\ln \left(\frac{\Delta_P}{\Delta_{AP}} \right) = 2 \frac{t_a^2 t_b^2}{h_{\text{ex}}^4} \left[7 \ln \left(\frac{h_{\text{ex}}}{\Delta_0} \right) - 4 - \ln \left(\frac{\Delta_0}{\eta} \right) \right], \quad (15)$$

where η is an ultra-violet cut-off. For weak ferromagnet we find⁹

$$\ln \left(\frac{\Delta_P}{\Delta_{AP}} \right) = 2 \frac{t_a^2 t_b^2}{\Delta_0^4} \left[\frac{3}{2} + \ln \left(\frac{4h_{\text{ex}}\eta}{\Delta_0^2} \right) \right] + 2 \frac{t_a^2 t_b^2 h_{\text{ex}}^2}{\Delta_0^6} \left[-\frac{19}{6} + 2 \ln \left(\frac{2h_{\text{ex}}^2}{\Delta_0 \eta} \right) \right] + \dots \quad (16)$$

4 Conclusions

We thus see that the perturbative expansions in the point contact geometry are rather different from the trilayers with atomic thickness: the small parameters are different, the divergencies are different. It was predicted for the point contact geometry that the self-consistent superconducting gap is larger in the parallel alignment⁷. This unusual feature of the proximity effect is present also in the atomic thickness geometry for half-metal ferromagnets⁸ and strong ferromagnets⁹. However the case of weak ferromagnets cannot be reproduced with the point contact geometry.

For weak ferromagnets we obtained non monotonic temperature dependences of the self-consistent superconducting gap for the F/S bilayer with atomic thickness⁹ and also with a finite thickness in the ferromagnetic and superconducting electrodes¹⁰. This unusual behavior is in agreement with the critical temperature obtained by solving linearized Usadel equations^{3,4}. This is related to Andreev bound states in the middle of the superconducting gap¹⁰. It also corresponds to the cross-over between the perturbation theory of strong ferromagnets in the high temperature regime (with $h_{\text{ex}} > \Delta_0$) and the perturbation theory of weak ferromagnets (with $h_{\text{ex}} < \Delta_0$) in the low temperature regime.

There are two differences between the point contact and atomic thickness geometries: the localized versus extended nature of the contact and the lateral confinement in the superconducting and ferromagnetic electrodes. A more complete investigation of the two factors will be presented elsewhere. We note here that from the study of F/S/F trilayers with a finite thickness¹⁰ we see that the non monotonic temperature dependence of the self-consistent superconducting gap exists if the width of the superconductor is smaller than the Fermi wave-length λ_F or larger than λ_F but smaller than the superconducting coherence length ξ_0 . The width of the superconductor is thus a critical parameter for the appearance of the specific regime of weak ferromagnets. If the width is larger than ξ_0 it can be conjectured that the the perturbation theory of the infinite planar geometry on Fig. 1-(b) can be deduced from the summation of the perturbation theories of a regular array of point contacts⁷. Finally geometrical effects were also investigated in a recent work¹¹ and the magnetization in the superconductor was calculated recently¹², in agreement with the atomic thickness geometry for strong ferromagnets. A more complete bibliography can be found elsewhere¹⁰.

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